CONVEX IS BACK: SOLVING BELIEF MDPS VIA CONVEXITY-INFORMED DEEP REINFORCEMENT LEARNING

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Abstract

We present a novel method for Deep Reinforcement Learning (DRL), incorporating the convex property of the value function over the belief space in Partially Observable Markov Decision Processes (POMDPs). We introduce hard- and softenforced convexity as two different approaches, and compare their performance against standard DRL on two well-known POMDP environments, namely the Tiger and FieldVisionRockSample problems. Our findings show that including the convexity feature can substantially increase performance of the agents, as well as increase robustness over the hyperparameter space, especially when testing on out-of-distribution domains.

1 INTRODUCTION

Markov Decision Processes (MDPs) have become the standard formalism for solving sequential decision making problems (Van Otterlo & Wiering, 2012). For applications in which perfect observability cannot be assumed, MDPs can be extended to model the probabilistic decision process as a Partially Observable MDP (POMDP), which provides an efficient framework for optimal decision making under uncertainty (Kochenderfer, 2015; Kaelbling et al., 1998; Shani et al., 2013; Braziunas, 2003; Walraven & Spaan, 2019; Oliehoek et al., 2008; Cassandra et al., 1994).

Classical dynamic programming (DP) and reinforcement learning RL are the two established solu-031 tion methods for MDP and POMDPs. RL approaches are used to overcome the curse of dimensionality of DP methods, and additionally do not require a model of the environment (Kochenderfer, 033 2015). Neural network (NN) based deep RL (DRL) applied to MDPs has been particularly success-034 ful, even in high dimensional problem settings (e.g., Mnih et al., 2013; 2015; Silver et al., 2016; 2018). Solving POMDPs is a more difficult task, but one approach is to directly handle the noisy observation-action history (or a variant thereof) (Koutas et al., 2024; Hettegger et al., 2023; Arcieri 037 et al., 2023). In cases, where no environment model is available, this is the only option. If one 038 has an environment model, then beliefs, i.e., a probability distribution over all system states, can be computed. Using beliefs can be computationally beneficial (Arcieri et al., 2023; Koutas et al., 2024); however, most current approaches do not use DRL with beliefs. In this work, we propose 040 to extend belief-based DRL solutions for POMDPs, by taking into account the theoretical property 041 that the optimal value function is convex over the belief space. We hypothesize that introducing this 042 informative property in the training process enables faster learning, and leads to better performance 043 in out-of-distribution (OOD) domains. 044

We propose two approaches for convexity-enforcement of the value function in the training process, namely soft-enforced and hard-enforced convexity. The performance of convexity-informed DRL is examined for both convexity approaches applied to the Dueling Q-Network (Wang et al., 2016) value-based architecture. Two benchmarks are used for performance comparison, which are the classic *Tiger* (Kaelbling et al., 1998) and *FieldVisionRockSample* (FVRS) (Ross et al., 2007) problems. We show that when trained with the convexity modification, the involved NNs have stronger generalization performance compared to the standard training schedule and, in some cases, better training performance.

053 Related work

Learning convex functions has a rich history in machine learning. However, the techniques devel-

oped in literature deal with explicitly defined target functions, e.g., including Karush-Kuhn-Tucker
 conditions of quadratic programs as differentiable layers Amos & Kolter (2017), log-likelihoods
 in conditional random fields Zheng et al. (2015), or energy functions in structured prediction en ergy networks Belanger & McCallum (2016). These methods are not applicable to DRL, where the
 value function is implicitly defined through the Bellman equation, and are thus not similar to our
 contribution.

060 Regarding hard-enforced convex NNs for MDP problems, the closest work to this paper is a com-061 bination of Amos et al. (Amos et al., 2017) and Sivaprasad et al. (Sivaprasad et al., 2021). Amos 062 et al. (Amos et al., 2017) introduce fully and partially input convex neural networks, where the 063 architectures include required skip connections at every layer. The focus of their work lies more on 064 performing inference on the final convex NN to find the optimal input values. Their reference to the application on DRL focuses merely on perfectly observable and continuous action problems. They 065 represent the negative Q-function with an input convex NN, and subsequently select the optimal ac-066 tion as a convex optimization problem over the NN output. However, they do not consider partially 067 observable environments, as is the focus of this work. Sivaprasad et al. (Sivaprasad et al., 2021) de-068 fine conditions to achieve input-output convexity with fully connected NNs without the need for skip 069 connections, and convolutional architectures; however, they do not consider DRL implementations.

Regarding soft-enforcement of convexity in NNs for MDPs or POMDPs, we are not aware of any related work.

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2 Belief MDP

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076 Markov Decision Processes (MDP) provide an efficient framework for finding optimal solutions 077 in sequential decision making problems, where the environment E is stochastic, the consequence of the agent's actions is probabilistic, and the state of the environment is known (Puterman, 2014). Partially observable MDPs (POMDPs) provide a natural extension, where the true environment state 079 is not perfectly known; instead the agent receives imperfect observations (Kochenderfer, 2015). The POMDP can be formulated as an MDP by replacing the system states $s_t \in S$ with the corresponding 081 belief $b(s_t) = p(s_t \mid o_{1:t}, a_{1:t-1})$, where $o_t \in \mathbb{O}$ and $a_t \in \mathbb{A}$ denote the received observation and action performed by the agent, respectively. As new information is available to the agent, 083 the new belief states can be obtained with Bayesian updating (Kochenderfer, 2015; Andriotis & 084 Papakonstantinou, 2019): 085

$$(s_{t+1}) = p(s_{t+1} \mid o_{t+1}, a_t, \mathbf{b}_t) = \frac{O(o_{t+1} \mid s_{t+1}, a_t)}{p(o_{t+1} \mid \mathbf{b}_t, a_t)} \sum_{s_t \in \mathbb{S}} T(s_{t+1} \mid s_t, a_t) b(s_t),$$
(1)

where O and T represent the observation and state transition probabilities, respectively, $p(o_{t+1}|\boldsymbol{b}_t, a_t)$ is the normalizing constant, and the belief vector \boldsymbol{b}_t of length $|\mathbb{S}|$ represents the collection of beliefs $b(s_t) \forall s \in \mathbb{S}$ (Andriotis & Papakonstantinou, 2019).

Based on the chosen action and the underlying true state of the environment, the agent receives a reward $r_t \in \mathbb{R}$ determined by the reward function $r(s_t, a_t)$, and the expected reward in a certain belief state can be obtained by $r(\boldsymbol{b}_t, a_t) = \sum_{s_t \in S} r(s_t, a_t)b(s_t)$. The decision-making rule, mapping beliefs to actions, is called policy $\pi(\boldsymbol{b}_t)^{-1}$. The total expected discounted reward, or *value function*, $V^{\pi}(\boldsymbol{b}_t)$, starting from \boldsymbol{b} at time t until the horizon h under the policy π is defined as (Walraven & Spaan, 2019; Andriotis & Papakonstantinou, 2019):

$$V^{\pi}(\boldsymbol{b}_{t}) = \mathbb{E}_{\boldsymbol{s}_{k} \sim T, \boldsymbol{a}_{k} \sim \pi, \boldsymbol{o}_{k} \sim O} \left[\sum_{k=t}^{h} \gamma^{k-t} r(\boldsymbol{b}_{k}, \boldsymbol{a}_{k}) \right],$$
(2)

where $\gamma < 1$ defines a discount factor. Similarly to Equation 2, one can define an *action-value* function, $Q^{\pi}(\mathbf{b}_t, a_t)$, which defines the value of taking action a at belief \mathbf{b} at time t until the horizon h under the policy π :

$$Q^{\pi}(\boldsymbol{b}_{t}, a_{t}) = \mathbb{E}_{s_{k} \sim T, a_{k} \sim \pi, o_{k} \sim O} \left[\sum_{k=t}^{h} \gamma^{k-t} r(\boldsymbol{b}_{k}, a_{k}) \middle| a_{t} \right].$$
(3)

¹We limit this work to deterministic policies, but an extension to stochastic policies is possible

The relationship between Equations 2 and 3 is $V^{\pi}(\boldsymbol{b}_t) = Q^{\pi}(\boldsymbol{b}_t, \pi(\boldsymbol{b}_t))$. Having the Q-values, the agent's policy can be easily extracted by:

$$\pi(\boldsymbol{b}_t) = \operatorname*{arg\,max}_{a_t \in \mathbb{A}} Q^{\pi}(\boldsymbol{b}_t, a_t). \tag{4}$$

The goal of the agent is to find the policy which maximizes the expected sum of discounted rewards. This optimal policy π^* maximizes the value and action-values at every time t:

$$V^{*}(\boldsymbol{b}_{t}) := V^{\pi}(\boldsymbol{b}_{t})|_{\pi=\pi^{*}} = \max_{\pi} V^{\pi}(\boldsymbol{b}_{t})$$
(5)

$$Q^{*}(\boldsymbol{b}_{t}, a_{t}) := Q^{\pi}(\boldsymbol{b}_{t}, a_{t})|_{\pi = \pi^{*}} = \max_{\pi} Q^{\pi}(\boldsymbol{b}_{t}, a_{t}), \tag{6}$$

where Q^* satisfies the recursive Bellman optimality condition (Cassandra et al., 1994):

$$Q^{*}(\boldsymbol{b}_{t}, a_{t}) = r(\boldsymbol{b}_{t}, a_{t}) + \gamma \sum_{\boldsymbol{b}_{t+1} \in \mathbb{B}} p(\boldsymbol{b}_{t+1} | \boldsymbol{b}_{t}, a_{t}) \max_{a_{t+1} \in \mathbb{A}} Q^{*}(\boldsymbol{b}_{t+1}, a_{t+1}).$$
(7)

The focus of this work revolves around an important property of the optimal POMDP value function, namely that it should be convex over the belief space (Kochenderfer, 2015). The different methods of enforcing this property are discussed in Section 4 and the application of the approaches to the Dueling architecture is discussed in Section 5.1.

DEEP REINFORCEMENT LEARNING

One can use the recursive formulation in Equation 7 to find the function Q^* , from which the op-timal policy can then be extracted. Dynamic programming variants, such as, e.g., value or policy iteration, perform the optimization by iterating over all possible combinations of (belief) states, ac-tions and observations (Kochenderfer, 2015). However, due to the super-exponential growth in the value function complexity (Hauskrecht, 2000), this approach is not feasible for larger state and ac-tion spaces. By contrast, Neural Networks as universal function approximators (Hanin, 2019) have proven to be effective even in large state and action spaces, which has motivated their use for ap-proximating V, Q, or π , in what is known as Deep Reinforcement Learning (DRL) (e.g., Andriotis & Papakonstantinou, 2019; Vinyals et al., 2019).

One of the most prominent architectures for DRL are Deep Q-Networks (DQNs) (Mnih et al., 2013), where the recursive Equation 7 is reformulated into the temporal difference (TD) mean-squared error (MSE) loss function:

where $y^{(i)}$ denotes an output sample of the NN and $\tilde{}$ always denotes the counterpart of the target NN, whose weights get updated periodically (Mnih et al., 2015):

 $MSE_t = \frac{1}{n_t} \sum_{i=1}^{n_t} \left| y^{(i)} - \tilde{y}^{(i)} \right|^2$

$$y^{(i)} = Q(\boldsymbol{b}_t^{(i)}, a_t^{(i)} \mid \theta)$$
(9)

(8)

$$\tilde{y}^{(i)} = r_t^{(i)} + \gamma \max_{a_{t+1}^{(i)} \in \mathbb{A}} \tilde{Q}(\boldsymbol{b}_{t+1}^{(i)}, a_{t+1}^{(i)} \mid \tilde{\theta}).$$
(10)

Note that the Q-values in Equations 9 and 10 are DRL approximations of the optimal Q-function in Equation 6, and the TD-MSE in Equation 8 is a sample-based approximation of the Bellman condition in Equation 7. The assumption is that, given enough samples and training, the DRL approximation should converge to the optimal solution.

CONVEX NEURAL NETWORKS

4.1 CONVEXITY CONDITIONS FOR MULTI-DIMENSIONAL FUNCTIONS

A function $f: \mathbb{R}^n \longrightarrow \mathbb{R}$ is convex if its domain is a convex set and for all u, v in its domain, and all $t \in [0, 1]$, we have (Ahmadi & Hall, 2016)

$$f(t\boldsymbol{u} + (1-t)\boldsymbol{v}) \le tf(\boldsymbol{u}) + (1-t)f(\boldsymbol{v})$$
(11)

162 If f is differentiable, one can define an alternative condition of convexity, which is equivalent to 163 Equation 11 (Ahmadi & Hall, 2016):

$$f(\boldsymbol{u}) + \nabla_{\boldsymbol{u}} f(\boldsymbol{u})^T (\boldsymbol{v} - \boldsymbol{u}) \le f(\boldsymbol{v}), \text{ for all } \boldsymbol{u}, \boldsymbol{v} \in \text{dom}(f).$$
(12)

166 If f is twice differentiable, the one can define yet another condition of convexity which is equivalent 167 to Equations 11 and 12 (Ahmadi & Hall, 2016):

$$0 \leq \boldsymbol{H}(f)(\boldsymbol{u}) = \nabla_{\boldsymbol{u}}^2 f(\boldsymbol{u}), \text{ for all } \boldsymbol{u} \in \operatorname{dom}(f),$$
(13)

i.e., the Hessian matrix H(f)(u) must be positive semi-definite. Equation 11 defines convexity in terms of the function value at different points, whereas Equations 12 and 13 define convexity via the first and second derivatives.

4.2 HARD-ENFORCED CONVEXITY

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The first obvious choice to satisfy convexity in the value function is to use an NN architecture which guarantees convexity. Considering a multi-layer perceptron of k layers, where $h_i^{(l)}$ denotes the *i*-th neuron output in the *l*-th layer, then for an input $x \in \mathbb{R}^d$, $h_i^{(l)}$ is defined as (Sivaprasad et al., 2021):

$$h_i^{(l)} = \phi\left(\sum_j W_{i,j}^{(l)} h_j^{l-1} + b_i^{(l)}\right),$$
(14)

with weights $W_{i,j}^{(l)}$, bias $b_i^{(l)}$ and activation function $\phi(x)$. Further, $h_j^{(0)} = x_j (j = 1, ..., d)$ and $h_j^{(k+1)} = y_j$ (*j*th NN output). Only two conditions are needed to ensure convexity of the final output y with respect to the input x, namely (Amos et al., 2017; Sivaprasad et al., 2021):

i)
$$0 \le W_{i,j}^{(2:k+1)}$$

ii) ϕ is convex and a non-decreasing function.

Condition ii) can be achieved by using, e.g., Leaky Rectified Linear Unit (LReLU) (Maas et al., 2013), Parametric ReLU (PReLU) (He et al., 2015) or Exponential LU (ELU) (Clevert et al., 2015) activation functions.

Condition i) needs to be enforced during the training process, e.g., by clipping negative weights to zero, taking absolute of weights, exponentiation of negative weights, or shifting negative weights after each iteration (Sivaprasad et al., 2021). As this enforcement from outside interferes with the weight updates, and hence potentially hinders training, we also investigate the approach of softenforced convexity. Note that other, more complex approaches exist to enforce convexity, e.g., by representing weights as separate NN layers with absolute activation functions (Rashid et al., 2020). However, this would change the underlying architecture and complicate comparability between the approaches, which is why other enforcement options are left for future research.

201 4.3 SOFT-ENFORCED CONVEXITY

Soft-enforced convexity mimics the idea of soft-enforced differential equations in Physics-Informed
 Neural Networks (PINNs) (Raissi et al., 2019). The core idea is to add a second term to the temporal loss function in Equation 8, which penalizes deviations of the target function from one of the convexity criteria outlined in Section 4.1. Suppose we use the MSE loss function also for the second term, then the total MSE loss function is:

$$MSE = MSE_t + c \cdot MSE_c, \tag{15}$$

where the constant c defines the relative weight of the TD- and convexity loss terms.

211 5 METHODOLOGY

- 213 5.1 CONVEXITY-INFORMED DRL
- The NN architecture used throughout this work is the Dueling architecture (Wang et al., 2016) depicted in Figure 1.

Figure 1: Dueling network architecture, with the belief input (black), dense layers (gray), value stream (cyan), advantage stream (green) and Q-value output (red). Arrows indicate dense weights and the brown lines indicate computation without weights; adapted from (Wang et al., 2016).

Hard-enforcement of the value-convexity with respect to the belief input is performed by adjusting
 the weights according to condition i) in Section 4.2 in the shared layers (gray), as well as the value
 stream (cyan) in Figure 1. Condition ii) in Section 4.2 is met by an appropriate choice of the
 activation function, which is kept identical for all layers.

Soft-enforcement of the value-convexity is performed by adding a second loss term according to Equation 15. Depending on the choice of the convexity criterion, namely point-based (p) in Equation 11, or gradient-based (g) in Equation 12, MSE_c takes the form of:

$$MSE_{c}^{p} = \frac{1}{n_{c}} \sum_{i=1}^{n_{c}} \max\left\{0, f(t^{(i)}\boldsymbol{u}^{(i)} + (1 - t^{(i)})\boldsymbol{v}^{(i)}) - t^{(i)}f(\boldsymbol{u}^{(i)}) - (1 - t^{(i)})f(\boldsymbol{v}^{(i)})\right\}^{2}$$
(16)

$$MSE_{c}^{g} = \frac{1}{n_{c}} \sum_{i=1}^{n_{c}} \max\left\{0, f(\boldsymbol{u}^{(i)}) + \nabla_{\boldsymbol{u}} f(\boldsymbol{u}^{(i)})^{T} (\boldsymbol{u}^{(i)} - \boldsymbol{v}^{(i)}) - f(\boldsymbol{v}^{(i)})\right\}^{2}.$$
 (17)

The hessian-based condition in Equation 13 cannot be translated into a loss function in a straightforward manner. A matrix M is positive semi-definite (psd) if

$$\boldsymbol{x}^T \boldsymbol{M} \boldsymbol{x} \ge 0 \quad \forall \boldsymbol{x} \in \mathbb{R}^n.$$
 (18)

For 1D inputs, this is not a problem and the condition reduces to $\frac{d^2}{du^2}f(u) \ge 0$ and the convex loss takes the form of

$$MSE_{c}^{h,1D} = \frac{1}{n_{c}} \sum_{i=1}^{n_{c}} \max\left\{0, -\frac{d^{2}}{du^{(i)^{2}}}f(u_{i})\right\}^{2}.$$
(19)

By contrast, for multidimensional inputs, Equation 18 can be checked in a sample based manner:

$$MSE_{c}^{h,nD} = \frac{1}{n_{c}} \sum_{i=1}^{n_{c}} \frac{1}{n_{psd}} \sum_{j=1}^{n_{psd}} \max\left\{0, -\boldsymbol{x}^{(j)^{T}} \boldsymbol{H}(f)(\boldsymbol{u}^{(i)})\boldsymbol{x}^{(j)}\right\}^{2}.$$
 (20)

 $u^{(i)}$ and $v^{(i)}$ in Equations 16, 17, 19 and 20 denote points $i = 1, ..., n_c$ sampled from the belief space, for which the respective convexity condition is checked; $x^{(j)}$, $j = 1, ..., n_{psd}$ denote points sampled from \mathbb{R}^n for which the psd condition in Equation 18 checked.

Conce the respective soft enforcement method is chosen, belief points $b^{(i)}$ (corresponding to $u^{(i)}$) are sampled from the problem-specific belief space and, together with other inputs, propagated through the network to obtain their values $V(b^{(i)})$ (corresponding to $f(u^{(i)})$). In this work, we employ the Dueling architecture, hence the values can be obtained by propagation through the shared layers (gray) and subsequently through the value stream (cyan) of the network in Figure 1.

5.2 NUMERICAL INVESTIGATIONS

269 With numerical experiments, we test if enforcing convexity in the value function can improve the performance of DRL. Specifically, we test the following two hypotheses:

H1: Enforcing convexity enables the DRL agent to learn faster due to restriction of the search space.

272 H2: Convexity-informed DRL performs better in out-of-distribution domains due to improved ex 273 trapolation of the value function.

The two hypotheses are tested with experiments on two classic problems, namely the *Tiger* (Kaelbling et al., 1998) and the *FieldVisionRockSample* (FVRS) (Ross et al., 2007) environments. Detailed descriptions of these problems are given in Sections C and D.

To test H1, we train the DRL agent with and without enforcing convexity for a fixed number of training steps. We then compare the performance of the individual agents.

279 To test H_2 , we evaluate the performance of the agents for belief points which are not included in 280 the training distribution. We achieve this by testing on observation functions which differ from the 281 one used to train the agent. For the Tiger problem, we simply change the constant Tiger observation 282 accuracy. For FVRS, the observation accuracy p_{obs} for a rock depends on its Euclidian distance d to 283 the agent. The default (def) observation function is given as $p_{obs}^{def}(d) = 0.5 + 2^{-1-d/d_0}$, where the 284 constant $d_0 = (n-1)\sqrt{2}/4$ is chosen depending on the grid size n. To evaluate the agent on OOD 285 data, we define the heaviside (heavi) function $p_{obs}^{heavi}(d) = 1$ for $d \le d_0$ else 0.5, where $d_0 = 1$. 286 Furthermore, we also define a set of constant (const) observation functions $p_{obs}^{const}(d) = c$, which do 287 not depend on the distance between rock and agent. We use $c \in \{0.5, 0.6, ..., 1.0\}$.

To allow for a fair comparison between the DRL with and without enforcing convexity we fix the 289 hyperparameter optimization procedure beforehand. This prevents bias inflicted during the opti-290 mization (e.g., amount of time invested, number of samples, amount of steps). The detailed proce-291 dure used is reported in Section E. After the hyperparameter search is conducted, we perform two 292 separate investigations. Firstly, we evaluate the performance of each method over all hyperparame-293 ter samples, yielding a rough estimate of the robustness/sensitivity of each method with respect to 294 changing hyperparameters. This approach is not customary in Machine Learning, which is why the 295 corresponding results are only reported in Section B. Secondly, we take the best hyperparameters 296 of each search, and evaluate them over a certain number of runs. The results of this conventional 297 approach are reported in the main text in Section 6.

The final policy of each agent is evaluated with a Monte Carlo (MC) approximation of the expected sum of discounted rewards \hat{s}_r . To evaluate the performance of each method, we employ boxplots, comprising the median, interquartile range, and maximum performance, which allows a more complete interpretation of the obtained results.

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6 Results

6.1 COMPUTATION TIME

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All computations were performed on an Nvidia Tesla V100 GPU with 16GB RAM. For the Tiger problem, training for 5,000 steps and evaluating the policy with $2 \cdot 10^5$ MC samples took around 5 minutes. For FVRS, training for 50,000 steps and evaluating the policy with 10^4 MC samples took approximately 60 minutes.

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6.2 TIGER

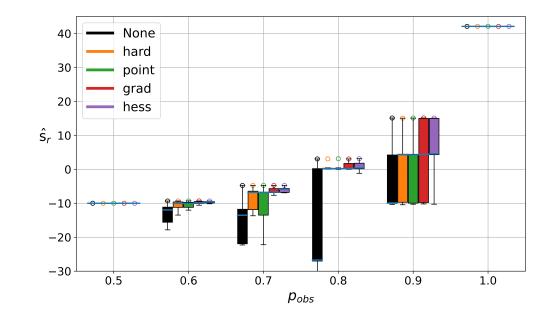
We test the Tiger problem for all versions of enforced convexity (hard, point, grad and hess) as well as for the standard approach without enforced convexity.

A visualization of the convexity violation of the standard DRL approach, as well as the corresponding value function correction of our proposed methods is shown in Section B.1.

We perform a hyperparameter search for all convexity methods for various observation accuracies $p_{obs} = \{0.6, 0.8, 0.9, 1.0\}$. The evaluation of our hypotheses over the whole hyperparameter search is outlined in Section B.1.

The test of H1 for the best hyperparameters yields no difference between the standard DRL approach and our proposed methods. This is due to the simplicity of the problem, where the majority of agents finds the optimal policy in the given amount of steps; thus, the mean performance over multiple seeds
 is close to the optimal performance with only little variation.

To test H_2 for the best hyperparameters, we train the agents on a specific observation accuracy 327 and cross-evaluate their performance on different observation accuracies. Since again, the major-328 ity of the hyperparameters converge to the optimal solution, we perform the cross-evaluation over all optimal agents. We observe that for agents trained on $p_{obs} = \{0.6, 0.8, 0.9\}$ there was no no-330 ticeable difference in the cross-evaluation performance between the individual convexity methods. 331 Our explanation for this is that the optimal policy is characterized by two transition points from the 332 action 'listen' to 'open-left'/'open-right'. Since these transition points lie very close to each other 333 for $p_{obs} \in (0.5, 1.0)$ the methods do not have to perform a large extrapolation, which leads to almost identical results. For $p_{obs} = 1.0$, however, the agent receives only the belief points b = 0.5334 and b = 1.0 during training; thus, the agent does not know the location of the policy transition. 335 For this case, the results are shown in Figure 2, where the performance on the originally trained 336 observation accuracy is the same for all agents (cf. H1), but the performance on $\{0.6, 0.8, 0.9\}$, in 337 a distributional sense, is noticeably worse for the plain DRL approach compared to all convexity-338 enforced methods. This is reflected by lower medians (blue lines) and/or worse interquartile ranges. 339 This shows that a well-behaved extrapolation of the value function can lead to better performance 340 in out-of-distribution domains. We note that the max over all optimal agents is still the same for all 341 methods. We suspect that this is again due to the simplicity of the Tiger problem. 342





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Figure 2: Boxplots (color-coded) over all optimal agents of a hyperparameter search with 200 runs for each convexity method. An optimal agent is one which has reached the optimal policy in the given amount of training steps, and the number of optimal agents was for grad: 178, hard: 68, hess: 69, None: 193, point: 183. The agents have been trained on $p_{obs} = 1.0$ and cross-evaluated on $p_{obs} = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ with 10^5 MC samples. Each boxplot includes the median as a blue horizontal line, interquartile range (IQR) as an opaque colored box, as well as the 1.5-IQR distances from the respective quartiles as whiskers; the maximum achieved value is marked with a colored hollow circle, other outliers are not visualized to avoid cluttering.

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6.3 FVRS

For FVRS, we do not consider the hard-enforced approach, because the value function is convex with regard to the belief inputs but not with regard to the position inputs. However, enforcing convexity of the neural network for only a subset of the inputs is not straightforward, hence we choose to leave this for further research. Moreover, we also do not consider the hessian approach to soft-enforced convexity. Computing second derivatives is simply too time-intensive for larger problems and one would choose other optimization algorithms (e.g., Newton) over gradient descent
 if second derivatives were available.

Furthermore, for FVRS we use the LReLU activation functions, as we noticed that during training when the method converges to a stable policy (e.g., always go left), the weights of the hidden layers become high and negative. This ensures that the output is always -1 after passing through multiple ELU layers which yields the same Q-value for every possible combination of inputs. As a result, the method is stuck in this local minimum. To avoid this saturation, we switch to LReLU activation functions for the FVRS problem.

Moreover, we do hyperparameter searches for all convexity methods for the default (def) and heaviside (heavi) observation functions. We report the performances on the originally trained environment as well as the cross-evaluations on other observation functions in the same figures. The results over all samples are reported in Section B.2, whereas the performances of the hyperparameters over 10 runs for are shown in Figures 3 and 4, respectively. When trained on the default setting (Figure 3), both convexity approaches perform better than standard DRL, both on the original and all OOD domains. On the other hand, when trained on the heaviside observation function, the gradient-based approach emerges as the single clear winner over all observation functions.

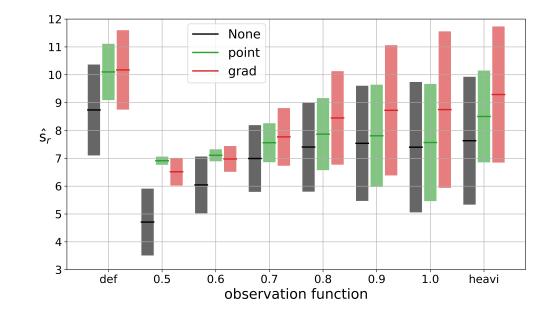


Figure 3: Best agents (color-coded) evaluated for 10 runs for each convexity method. The agents have been trained on the **default** observation function and are cross-evaluated on the heaviside (heavi) and a set of $p_{obs} = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ constant observation functions with 10^4 MC samples. The figure shows the respective reward means (solid horizontal line) as well as ± 1 standard deviation (transparent bars).

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7 CONCLUSION AND FUTURE WORK

In this work, we propose to extend DRL by enforcing the belief-convexity of the value function in the training process. We have shown that convexity-enforced DRL can yield notable improvements compared to the standard approach, such as better robustness over the hyperparameter space, as well as better mean performance of the best hyperparameters. Our approach performs particularly well when trained on edge case problems ($p_{obs} = 1.0$ for Tiger and $p_{obs} =$ heavi for FVRS) and applying the policy to the standard problem formulation counterpart. This suggests that a wellbehaved extrapolation of the value function leads to better policies when encountering OOD-data.

Based on the results in this work, we recommend the usage of the gradient-based enforcement, as
 it was better or at least equally good compared to the standard and point-based approach in every investigated setting.

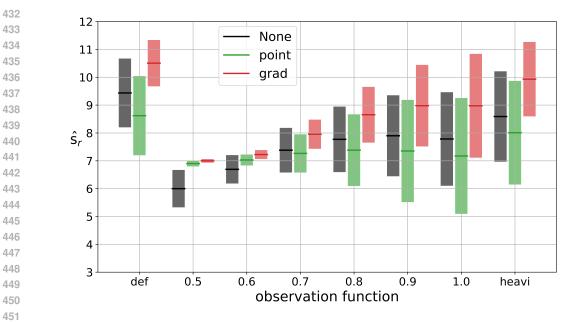


Figure 4: Best agents (color-coded) evaluated for 10 runs for each convexity method. The agents have been trained on the heaviside observation function and are cross-evaluated on the default (def) and a set of $p_{obs} = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ constant observation functions with 10⁴ MC samples. The figure shows the respective reward means (solid horizontal line) as well as ± 1 standard 455 deviation (transparent bars). 456

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458 Several new empirical results are presented in this paper, yet there are still numerous open questions 459 to be addressed. In particular, the largest performance gains of the convexity-enforced methods 460 have been observed when training on edge cases, and extrapolating to the standard settings. This 461 strongly suggests that these methods can improve performance when large extrapolations are needed. 462 Hence, we anticipate particularly promising future research directions to be for cases where value extrapolations are required, i.e., in low data regimes, and higher dimensional problems. On the other 463 hand, sampling-based techniques, as our soft-enforced methods, can face scalability challenges. 464 Further investigations of the application to high-dimensional belief spaces are needed to fully grasp 465 the potential of our proposed approaches. 466

467 Other potential research directions could be the investigation of convexity-informed DRL using actor-critic architectures, where the target directly is the value function, or the application of these 468 methods to continuous-state POMDPs. Further developments of the convexity injection, e.g., heuris-469 tics for choosing an optimal value for c in Equation 15, dynamic c adjustments along the lines of 470 LR-schedules, or including convexity loss every k training steps to speed up the training process, 471 can potentially lead to further improvements and training stability. 472

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8 **REPRODUCIBILITY STATEMENT**

476 For reproducibility, the source code for the environment, agent, as well as the configuration file 477 containing all relevant parameters is available at the provided website address in the first comment towards the reviewers. 478

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486	REFERENCES
487	

488	AA Ahmadi and G Hall. Theory of convex functions. Princeton University, Lecture, 7, 2016.
489 490 491	Brandon Amos and J Zico Kolter. Optnet: Differentiable optimization as a layer in neural networks. In <i>International conference on machine learning</i> , pp. 136–145. PMLR, 2017.
492 493	Brandon Amos, Lei Xu, and J Zico Kolter. Input Convex Neural Networks. In International Con- ference on Machine Learning, pp. 146–155. PMLR, 2017.
494 495 496 497	CP Andriotis and KG Papakonstantinou. Managing engineering systems with large state and ac- tion spaces through deep reinforcement learning. <i>Reliability Engineering & System Safety</i> , 191: 106483, 2019.
498 499 500	Giacomo Arcieri, Cyprien Hoelzl, Oliver Schwery, Daniel Straub, Konstantinos G Papakonstanti- nou, and Eleni Chatzi. POMDP inference and robust solution via deep reinforcement learning: An application to railway optimal maintenance. <i>arXiv preprint arXiv:2307.08082</i> , 2023.
501 502 503	David Belanger and Andrew McCallum. Structured Prediction Energy Networks. In International Conference on Machine Learning, pp. 983–992. PMLR, 2016.
504 505 506	James Bergstra and Yoshua Bengio. Random Search for Hyper-Parameter Optimization. <i>Journal of Machine Learning Research</i> , 13(2), 2012.
507	Darius Braziunas. POMDP solution methods. University of Toronto, 2003.
508 509 510	Anthony R Cassandra, Leslie Pack Kaelbling, and Michael L Littman. Acting Optimally in Partially Observable Stochastic Domains. In <i>AAAI</i> , volume 94, pp. 1023–1028, 1994.
511 512	Antony R. Cassandra. pomdp-solve, 2022. URL https://www.pomdp.org/code/. Accessed 08-December-2023.
513 514 515	Djork-Arné Clevert, Thomas Unterthiner, and Sepp Hochreiter. Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs). <i>arXiv preprint arXiv:1511.07289</i> , 2015.
516 517 518 519	Michael Hahsler and Hossein Kamalzadeh. POMDP: Introduction to Partially Observable Markov Decision Processes, 05 2021. URL https://cran.r-project.org/web/packages/ pomdp/vignettes/POMDP.html#the-tiger-problem-example. Accessed 08- December-2023.
520 521 522	Boris Hanin. Universal Function Approximation by Deep Neural Nets with Bounded Width and ReLU Activations. <i>Mathematics</i> , 7(10):992, 2019.
523 524	Milos Hauskrecht. Value-Function Approximations for Partially Observable Markov Decision Processes. <i>Journal of Artificial Intelligence Research</i> , 13:33–94, 2000.
525 526 527 528	Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification. In <i>Proceedings of the IEEE International</i> <i>Conference on Computer Vision</i> , pp. 1026–1034, 2015.
529 530 531 532	Daniel Hettegger, Carmen Buliga, Florian Walter, Elizabeth Bismut, Daniel Straub, and Alois Knoll. Investigation of Inspection and Maintenance Optimization with Deep Reinforcement Learning in Absence of Belief States. In 14th International Conference on Applications of Statistics and Probability in Civil Engineering, ICASP14, 2023.
533 534 535	Leslie Pack Kaelbling, Michael L Littman, and Anthony R Cassandra. Planning and acting in partially observable stochastic domains. <i>Artificial Intelligence</i> , 101(1-2):99–134, 1998.
536 537	Diederik P Kingma and Jimmy Ba. Adam: A Method for Stochastic Optimization. <i>arXiv preprint arXiv:1412.6980</i> , 2014.
538 539	Mykel J Kochenderfer. <i>Decision Making Under Uncertainty: Theory and Application</i> . MIT press, 2015.

540 541 542	Daniel Koutas, Elizabeth Bismut, and Daniel Straub. An investigation of belief-free DRL and MCTS for inspection and maintenance planning. <i>Journal of Infrastructure Preservation and Resilience</i> , 5(1):6, 2024.
543	5(1).0, 202
544 545	Andrew L Maas, Awni Y Hannun, Andrew Y Ng, et al. Rectifier Nonlinearities Improve Neural Network Acoustic Models. In <i>Proc. ICML</i> , volume 30, pp. 3. Atlanta, GA, 2013.
546	Volodymyr Mnih, Koray Kavukcuoglu, David Silver, Alex Graves, Ioannis Antonoglou, Daan Wier-
547	stra, and Martin Riedmiller. Playing Atari with Deep Reinforcement Learning. arXiv preprint
548	arXiv:1312.5602, 2013.
549	
550	Volodymyr Mnih, Koray Kavukcuoglu, David Silver, Andrei A Rusu, Joel Veness, Marc G Belle-
551	mare, Alex Graves, Martin Riedmiller, Andreas K Fidjeland, Georg Ostrovski, et al. Human-level
552	control through deep reinforcement learning. Nature, 518(7540):529-533, 2015.
553 554 555	Frans A Oliehoek, Matthijs TJ Spaan, and Nikos Vlassis. Optimal and Approximate Q-value Func- tions for Decentralized POMDPs. <i>Journal of Artificial Intelligence Research</i> , 32:289–353, 2008.
556	Martin L Puterman. Markov Decision Processes: Discrete Stochastic Dynamic Programming. John
557	Wiley & Sons, 2014.
558	
559	Maziar Raissi, Paris Perdikaris, and George E Karniadakis. Physics-Informed Neural Networks: A
560	Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial
561	Differential Equations. Journal of Computational Physics, 378:686–707, 2019.
562	Tabish Rashid, Mikayel Samvelyan, Christian Schroeder De Witt, Gregory Farquhar, Jakob Fo-
563	erster, and Shimon Whiteson. Monotonic Value Function Factorisation for Deep Multi-Agent
564	Reinforcement Learning. Journal of Machine Learning Research, 21(178):1–51, 2020.
565	g
566	Sashank J Reddi, Satyen Kale, and Sanjiv Kumar. On the Convergence of Adam and Beyond. arXiv
567	preprint arXiv:1904.09237, 2019.
568	Stéphane Ross, Brahim Chaib-Draa, et al. AEMS: An Anytime Online Search Algorithm for Ap-
569 570	proximate Policy Refinement in Large POMDPs. In <i>IJCAI</i> , pp. 2592–2598, 2007.
571 572	Guy Shani, Joelle Pineau, and Robert Kaplow. A survey of point-based POMDP solvers. Autonomous Agents and Multi-Agent Systems, 27(1):1–51, 2013.
573	Lavanya Shukla. Bayesian Hyperparameter Optimization - A Primer, 11
574	2023. URL https://wandb.ai/wandb_fc/articles/reports/
575	Bayesian-Hyperparameter-Optimization-A-PrimerVmlldzo1NDQyNzcw.
576	Accessed 15-Dezember-2023.
577	
578	David Silver, Aja Huang, Chris J Maddison, Arthur Guez, Laurent Sifre, George Van Den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, et al. Mastering
579	the game of Go with deep neural networks and tree search. <i>Nature</i> , 529(7587):484–489, 2016.
580	are game of 50 with deep neural networks and the search. $Nature$, $325(1501)$, $to 1 - 409$, 2010.
581	David Silver, Thomas Hubert, Julian Schrittwieser, Ioannis Antonoglou, Matthew Lai, Arthur Guez,
582	Marc Lanctot, Laurent Sifre, Dharshan Kumaran, Thore Graepel, et al. A general reinforcement
583	learning algorithm that masters chess, shogi, and Go through self-play. Science, 362(6419):1140-
584	1144, 2018.
585	Sorath Siyanrosod Ankur Singh Narash Manyani and Vingat Candhi. The Curious Case of Comment
586	Sarath Sivaprasad, Ankur Singh, Naresh Manwani, and Vineet Gandhi. The Curious Case of Convex Neural Networks. In <i>Machine Learning and Knowledge Discovery in Databases. Research Track:</i>
587	European Conference, ECML PKDD 2021, Bilbao, Spain, September 13–17, 2021, Proceedings,
588	<i>Part I 21</i> , pp. 738–754. Springer, 2021.
589	, rr
590	Trey Smith and Reid Simmons. Heuristic Search Value Iteration for POMDPs. arXiv preprint
591	arXiv:1207.4166, 2012.
592	Martin Van Ottanla and Marga Winning Dainforgeneert Learning and Marten Desi in D
593	Martijn Van Otterlo and Marco Wiering. Reinforcement Learning and Markov Decision Processes. In <i>Reinforcement Learning: State-of-the-Art</i> , pp. 3–42. Springer, 2012.

594 595 596 597	Oriol Vinyals, Igor Babuschkin, Wojciech M Czarnecki, Michaël Mathieu, Andrew Dudzik, Juny- oung Chung, David H Choi, Richard Powell, Timo Ewalds, Petko Georgiev, et al. Grandmaster level in StarCraft II using multi-agent reinforcement learning. <i>Nature</i> , 575(7782):350–354, 2019.
598 599	Erwin Walraven and Matthijs TJ Spaan. Point-Based Value Iteration for Finite-Horizon POMDPs. Journal of Artificial Intelligence Research, 65:307–341, 2019.
600 601 602	Ziyu Wang, Tom Schaul, Matteo Hessel, Hado Hasselt, Marc Lanctot, and Nando Freitas. Duel- ing Network Architectures for Deep Reinforcement Learning. In <i>International Conference on</i> <i>Machine Learning</i> , pp. 1995–2003. PMLR, 2016.
603 604 605 606 607	Shuai Zheng, Sadeep Jayasumana, Bernardino Romera-Paredes, Vibhav Vineet, Zhizhong Su, Da- long Du, Chang Huang, and Philip HS Torr. Conditional random fields as recurrent neural net- works. In <i>Proceedings of the IEEE international conference on computer vision</i> , pp. 1529–1537, 2015.
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648 A CONVEXITY VIOLATION

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To check whether the convexity violation of the standard approach is prevalent during training, we plot the value function of 6 example agents trained on the Tiger problem with $p_{obs} = 1.0$ in A.1. Note that not all None-based value functions showed convexity violations, but the majority.

To show that the convexity enforcement approaches proposed in this work mitigate the convexity violations, we also plot the value function of 6 example agents trained on the same setting, but now with gradient-based enforcement. The choice for gradient-based enforcement is arbitrary, all other proposed methods show similar convexity corrections.

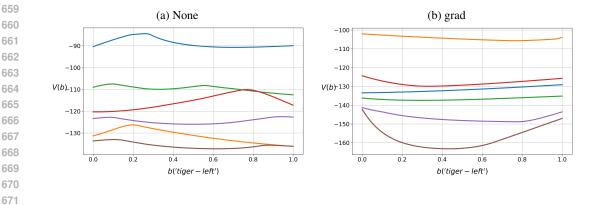


Figure A.1: Tiger value function plot over the belief space for 6 example agents trained without (a) and with gradient-based convexity enforcement (b) on $p_{obs} = 1.0$.

B ROBUSTNESS OVER HYPERPARAMETER SPACE

B.1 TIGER

680 To test H1 over all hyperparameters, we show their achieved reward distributions for observation 681 accuracies $p_{obs} = \{0.6, 0.8, 0.9, 1.0\}$ in Figure B.1. The figure shows that, in a distributional sense, 682 the performance is significantly worse for the hard-enforced and hessian soft-enforced convexity. 683 Our explanation for this is that training is harder with these convexity enforcements. For the hard enforcement, we suspect that the additional adjustment of the weights after the backpropagation 684 step, which assures that the output of the NN is convex with respect to the input, interferes with the 685 training and hence it is harder to find the optimal policy. For the hessian enforcement, we suspect 686 that calculating third order derivatives is not as stable, which results in slower learning. 687

B.2 FVRS

The results for all agents trained on the default, and cross-evaluated on the heaviside and constant observation functions, are shown in Figure B.2. The grad- and point-based methods perform better in all settings compared to the standard approach in terms of their medians and third quartiles (Q_3) . Note however, that the point method partially shows high variation, which is reflected by low first quartiles (Q_1) . Overall the grad method shows the best performance based on highest $Q_1 - Q_3$ (highest maximum performance is investigated in Section 6.3).

Even more pronounced is the difference when more extrapolation capacities are needed, i.e., when
training on the heaviside and evaluating on default and constant observation functions. The results
for this setting are shown in Figure B.3, where the best agents of the grad and point approaches
clearly perform better than the None counterpart, both on the original and OOD domains. There
does not seem to be a clear difference when comparing the medians of point and None; grad however
emerges as the clear best over all observation functions.

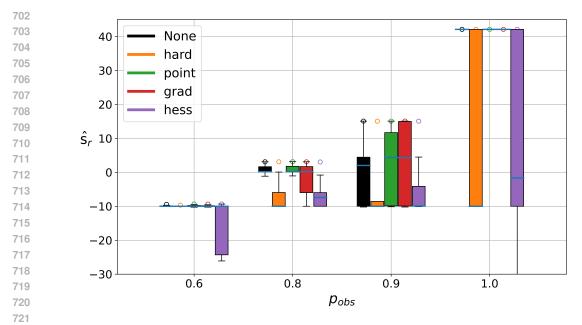


Figure B.1: Boxplots (color-coded) over all agents of a hyperparameter search with 200 runs for 722 each convexity method trained on $p_{obs} = \{0.6, 0.8, 0.9, 1.0\}$, and evaluated with 10^5 MC samples. 723 Each boxplot includes the median as a blue horizontal line, interquartile range (IQR) as an opaque 724 colored box, as well as the 1.5-IQR distances from the respective quartiles as whiskers; the maximum 725 achieved value is marked with a colored hollow circle, other outliers are not visualized to avoid 726 cluttering. 727

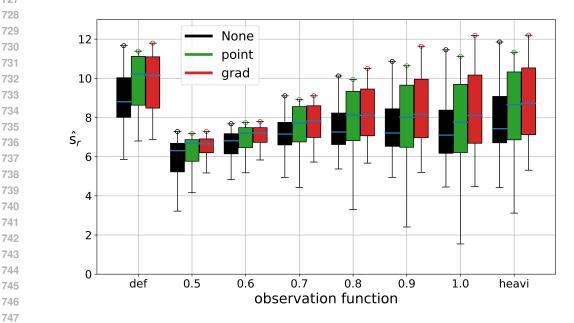


Figure B.2: Boxplots (color-coded) over all agents of a hyperparameter search with 150 runs for 748 each convexity method. The agents have been trained on the default (def) observation function and 749 are cross-evaluated on the heaviside (heavi) and a set of $p_{obs} = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ constant 750 observation functions with 10^4 MC samples. Each boxplot includes the median as a blue horizontal 751 line, interquartile range (IQR) as an opaque colored box, as well as the 1.5-IQR distances from 752 the respective quartiles as whiskers; the maximum achieved value is marked with a colored hollow 753 circle, other outliers are not visualized to avoid cluttering. 754

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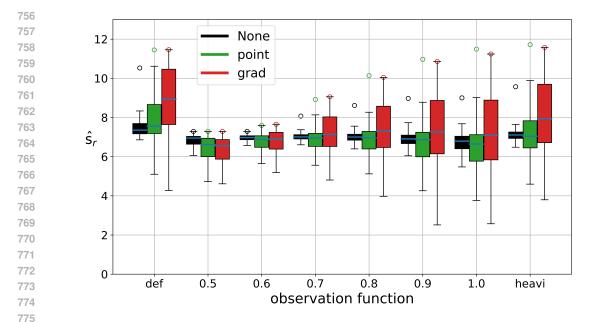


Figure B.3: Boxplots (color-coded) over all agents of a hyperparameter search with 150 runs for each convexity method. The agents have been trained on the **heaviside** (heavi) observation function and are cross-evaluated on the default (def) and a set of $p_{obs} = \{0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$ constant observation functions with 10⁴ MC samples. Each boxplot includes the median as a blue horizontal line, interquartile range (IQR) as an opaque colored box, as well as the 1.5 IQR distances from the respective quartiles as whiskers; the maximum achieved value is marked with a colored hollow circle, other outliers are not visualized to avoid cluttering.

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C TIGER PROBLEM

786 C.1 TIGER DESCRIPTION

The Tiger problem (Kaelbling et al., 1998) consists of an agent standing in front of two doors. Behind one of the doors there is a tiger (T), behind the other there is no tiger (\overline{T}) , and the agent does not know where the tiger is. At each timestep the agent can decide whether he wants to open one of the doors with the actions 'open-right' / 'open-left' (O^R / O^L) or perform a listening (L) action. By listening, the agent hears the tiger roaring behind its true location with probability $p_{obs} \in [0.5, 1.0]$.

Opening the door with the tiger behind yields a reward of r(T) = -100, opening the other door incurs $r(\bar{T}) = 10$. Listening on the other hand, costs r(L) = -1. After opening a door, the environment resets with a new random tiger location.

796 The environment state of the Tiger problem can be fully described with a scalar value denoting, e.g., the belief of the tiger being behind the left door $b \in [0.0, 1.0]$. In general, the optimal policy depends 797 on the horizon h, i.e., the number of times the game is played. For the special cases of h = 1 and 798 $h \to \infty$, the optimal policy collapses to a relatively simple one. It consists of listening at every 799 timestep until the belief that the tiger is at a given door falls below a certain optimal belief threshold 800 b_{opt} , or the belief surpasses $1 - b_{opt}$. For h = 1, the associated optimal belief threshold b_{opt}^1 can be 801 obtained by considering only the immediate expected rewards. The agent should open the door if 802 the associated expected reward is higher than the expected reward of listening: 803

$$\mathbb{E}\left[\mathbf{r}(b, O^{R/L})\right] > \mathbb{E}\left[\mathbf{r}(b, L)\right]$$

$$\iff \quad b(T)r(T) + (1 - b(T))r(\bar{T}) > r(L) \tag{21}$$

$$\iff \quad b(T) < \frac{r(L) - r(\bar{T})}{r(T) - r(\bar{T})} = b_{opt}^{1}.$$

With the aforementioned rewards, $b_{opt}^1 = 0.1$.

Table C.1: Optimal Q-values for beliefs $b^S = 0.5$, $b^L = 1.0$, $b^R = 0.0$ and actions L, O^L , O^R for horizon $h \to \infty$ and r_{PO}^* given in Equation 26.

813			
814		O^L	O^R
815	$b^S r_{PO}^*$	$-45 + \gamma r_{PO}^*$	$-45 + \gamma r_{PO}^*$
816	$b^L \mid r_{PO}^*$	$-100 + \gamma r_{PO}^{*}$	$10 + \gamma r_{PO}^{*}$
817	$b^R \mid r_{PQ}^*$	$10 + \gamma r_{PO}^*$	$-100 + \gamma r_{PO}^{*}$
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820 For $h \to \infty$, the derivation of the thresholds is generally not trivial, as the discounted expected 821 reward of future games has to be considered in addition to the immediate reward, and the threshold 822 depends on the observation accuracy. Thus, we use the *pomdp* package, which is an R implemen-823 tation of the well-known original pomdp-solve developed by Antony Cassandra (Cassandra, 2022; 824 Hahsler & Kamalzadeh, 2021). Instead of calculating the thresholds, we extract the optimal policy graphs together with the associated belief points and optimal expected rewards achieved with dis-825 count factor $\gamma = 0.9$ for the investigated observation accuracy cases. Computing the KL-divergence 826 of the optimal policy graphs and the agent policies gives a faster way of determining whether the 827 optimal policy is reached than with extensive MC simulation. 828

In Sections C.2 and C.3 some special cases resulting from this general optimal policy are outlined, for which the optimal rewards and Q-values can be calculated analytically.

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C.2 UNINFORMATIVE OBSERVATIONS

834 When $p_{obs} = 0.5$, listening does not yield an improvement of the initial belief (hence, the explored 835 belief space reduces to a single point $b^S = 0.5$). Here, the optimal action is to listen at every 836 timestep and the optimal reward r_{UI}^* and optimal Q-values $Q^*(b, a_i)$ depending on the horizon h837 and discount factor γ are:

$$r_{UO}^* = -\sum_{t=0}^h \gamma^t = -\frac{1-\gamma^{h+1}}{1-\gamma} \stackrel{h \to \infty}{=} -\frac{1}{1-\gamma}$$
(22)

$$Q^*(b,L) = r_{UO}^*$$
(23)

$$Q^*(b^S, O^L) = 0.5 \cdot 10 + 0.5 \cdot (-100) - \sum_{t=1}^h \gamma^t$$

$$= -45 - \gamma \frac{1 - \gamma^h}{1 - \gamma} \stackrel{h \to \infty}{=} -45 - \frac{\gamma}{1 - \gamma}$$
(24)

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$$Q^*(b^S, O^R) = Q^*(b^S, O^L)$$
(25)

C.3 PERFECT OBSERVATIONS

When $p_{obs} = 1.0$, listening once directly yields the position of the tiger with certainty. Here, the optimal policy is to listen first and then to open the door opposite to the perceived roar. The optimal reward r_{PO}^* and optimal Q-values for belief states $b^S = 0.5$, $b^L = 1.0$, $b^R = 0.0$ depending on the trajectory until horizon h and discount factor γ are given in Equations 26 and C.1

$$r_{PO}^{*} = -1 + 10\gamma - \dots + 10\gamma^{h} = -\sum_{t=0}^{\frac{h-1}{2}} \gamma^{2t} + 10 \sum_{t=0}^{\frac{h-1}{2}} \gamma^{2t+1}$$

$$= -\frac{1-\gamma^{h+1}}{1-\gamma^{2}} + 10 \frac{1-\gamma^{h+2}}{1-\gamma^{2}} \stackrel{h \to \infty}{=} \frac{10\gamma - 1}{1-\gamma^{2}}.$$
(26)

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864 D FVRS PROBLEM

866 D.1 FVRS DESCRIPTION

The FieldVisionRockSample (Smith & Simmons, 2012; Ross et al., 2007) problem is defined by a tuple (n, k), where *n* defines the width of a square grid and *k* the number of rocks distributed randomly in the grid. The state of each rock is either good (GR) or bad (BR). The actions available to the agent at each timestep are to move north (MN), south (MS), east (ME), west (MW), or to perform a sampling (C) action. The starting point of the agent is randomly sampled along the west boundary of the grid, and there is an exit zone situated along the east boundary of the grid.

874 Upon reaching the exit zone the agent receives the reward $r_E = 10$. When the agent is located in the same grid cell as a rock, it can sample it. If the rock is good, the agent receives $r_{GR} = 10$; if 875 it is bad, the agent receives $r_{BR} = -10$. Otherwise, performing the sampling action with no rock 876 present incurs a reward of 0. In addition, we punish the agent if it wants to move out of the grid at the 877 west, north and south boundary. These illegal moves are associated with a reward of $r_{IM} = -10$. 878 Hence overall, in order to maximize the expected sum of discounted rewards, the task of the agent 879 is to sample good rocks and to reach the exit zone in as few steps as possible. Throughout this work 880 we use (n, k) = (4, 4). 881

882 D.2 BELIEF UPDATE

The standard belief update after on observation is given in Equation 1. Firstly, the dependence of O on action a_t can be dropped, since the observations only depend on the state of the rocks and their distance to the robot. Furthermore, an action does not change the state of the rocks², thus the transition probabilities reduce to $T(s_{t+1}, s_t) = \delta_{t+1,t}$, where $\delta_{t+1,t}$ denotes the Kronecker delta. Hence, the belief update can be simplified to

$$b(s_{t+1}) \propto O(o_{t+1} \mid s_{t+1}) b(s_t).$$
(27)

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The first obvious stationary policy is if the agent completely ignores the rocks and collects the exit reward as fast as possible. Thus, the policy consists of choosing the action *"move east"* at every timestep the reward resulting from this policy is

$$r^* = \gamma^{n-1} r_E. \tag{28}$$

The optimal Q-values under the policy of only moving east are then independent of the rock positions as well as the belief about the rock states, i.e., they only depend on the on the position of the agent relative to the exit zone. To simplify, we can formulate an averaged optimal Q-value $\tilde{Q}^*(A) = \mathbb{E}_B[Q^*(b, A)]$ by averaging over all grid positions.

$$\tilde{Q}^{*}(ME) = \frac{\gamma^{0}r_{E} + \gamma^{1}r_{E} + \dots + \gamma^{n-1}r_{E}}{n} = \frac{r_{E}}{n}\sum_{t=0}^{n-1}\gamma^{t} = \frac{1-\gamma^{n}}{1-\gamma}\frac{r_{E}}{n}.$$
(29)

Likewise, for actions MN, MS, MW we have to take into account the delay of exit reward as well as potential negative rewards incurred due to illegal moves at the borders. Similarly, for action C, we have to consider the delay of exit reward as well as the expected reward for performing action C at the agent's location. Since, in our case, the rocks are equally likely to be in a good or a bad state(p(GR) = p(BR)), the rewards for a good and bad rock have the same absolute value $r_{GR} = -r_{BR}$, and the reward for performing action C when there is no rock is 0, the overall expected collection reward is zero:

$$\mathbb{E}\left[\mathbf{r}(C)\right] = \mathbf{r}(C|R)p(R) + \mathbf{r}(C|\bar{R})p(\bar{R})$$

$$= \frac{k}{n^2}\left[p(GR)r_{GR} + p(BR)r_{BR}\right] + \frac{n^2 - k}{n^2}\mathbf{r}(C|\bar{R})$$

$$= 0.$$
(30)

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²To be precise, sampling a good rock does change its state to a bad rock; this is however implemented as an additional step after the belief update and hence can be ignored here

918 Hence, the averaged optimal Q-values for each action are

$$\tilde{Q}^{*}(MN) = \frac{r_{E}}{n} \sum_{t=1}^{n} \gamma^{t} + \frac{r_{IM}}{n} = \gamma \tilde{Q}^{*}(ME) + \frac{r_{IM}}{n}$$
(31)

$$\tilde{Q}^*(MS) = \tilde{Q}^*(MN) \tag{32}$$

$$\tilde{Q}^{*}(MW) = \frac{r_{E}}{n} \sum_{t=2}^{n+1} \gamma^{t} + \frac{r_{IM}}{n} = \gamma^{2} \tilde{Q}^{*}(ME) + \frac{r_{IM}}{n}$$
(33)

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$$\tilde{Q}^*(C) = \gamma \tilde{Q}^*(ME). \tag{34}$$

929 D.4 CONVENIENCE COLLECTION POLICY

Another stable policy with higher reward than completely ignoring the rocks would be to keep moving towards the exit zone at every timestep. However, if a good rock lies incidentally on the path of the agent, it is collected. This policy is always better or equal than ignoring the rocks, when the rewards are selected as

$$\gamma^{n-1}r_E \le \gamma^n r_E + \gamma^{n-1}r_{GR} \quad \longrightarrow \quad (1-\gamma)\,r_E \le r_{GR},\tag{35}$$

which is guaranteed by the initial setup. To calculate the analytical reward and Q-values resulting from this policy is not straightforward, but can be easily obtained with Monte Carlo simulation.

E TRAINING SPECIFICATIONS

941 We first start with a large number of hyperparameters and a broad range (i.e., multiple orders of 942 magnitude) of possible values. For each convexity method, we then sample this space of possible 943 hyperparameters with a fixed number of samples, which we call training runs, and let the agents train for a fixed number of timesteps (no early stopping). The sampling of the hyperparameter space 944 is conducted via via Bayesian hyperparameter tuning (Shukla, 2023), which empirically finds better 945 hyperparameters compared to their more prominent counterparts, namely grid and random search 946 (Bergstra & Bengio, 2012). At the end of each run, we evaluate the policies of the respective agents. 947 In the general case, we estimate the achieved expected sum of discounted rewards with Monte Carlo 948 simulation. For the Tiger problem, an optimal solution is available with classical methods; hence, we 949 can additionally use the Kullback-Leibner divergence to filter for agents which achieved the optimal 950 policy (e.g., in Figure 2). 951

Since the agents usually find the optimal solution when trained for a sufficiently large number of steps, we heavily restrict the number of available steps for each training run. A few training runs were used for an initial estimate of the speed of convergence and a fraction of that was used for the cutoff. Based on this small pre-analysis, the maximum number of training steps is chosen as 5,000 and 50,000 for the Tiger and FVRS problems, respectively.

For the Tiger problem, we consider the infinite-horizon stationary policy. With a discount factor of $\gamma = 0.9$, the rollout depth d_T was chosen as 150, where the reward's contribution to the sum of discounted rewards is in the order of 10^{-5} . On the other hand, for the FVRS problem, we search for the policy which maximizes the expected rewards over a game instance, i.e., from the starting point until the robot reaches the end zone. We restrict the maximum rollout depth to $d_{FVRS} = n^2 \cdot k$. Hence, this defines a limit policy of visiting every grid cell and sampling every rock.

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F NEURAL NETWORK SPECIFICATIONS

For this work, we fixed a number of network and optimizer parameters, the specifications can be
found in Tables F.1 and F.2. Unless otherwise specified, we use the PyTorch default values. The
resulting total number of trainable weights for the Tiger and FVRS networks are given as 174 and
32,106, respectively.

970 On the other hand, a number of parameters are selected to be optimized. We choose the Bayesian 971 optimization method with an MC approximation of the expected sum of discounted rewards evaluated at the end of each training run as the maximization target. We reduce the learning rate when

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5	Parameter	Tiger/FVRS value
	Architecture type	Dueling (Wang et al., 2016)
	Target update type	hard
	Target update period	3
	Batch size	20
	Rollout steps	25
	Discount factor γ	0.9
	Optimizer	Adam (Kingma & Ba, 2014)
	AMSGRAD	Included (Reddi et al., 2019)
	Minimum learning rate	10^{-4}
	Initial exploration rate	0.5

Table F.1: Environment-independent fixed network and optimizer parameters

Table F.2: Environment-specific fixed network and optimizer parameters

Parameter	Tiger	FVRS
# input nodes	1	3k+2
# output nodes	3	5
# FC Layer	2	3
FC layer width	10	100
# value layers	-	1
Lalue layer width	-	50
# advantage layers	-	1
Advantage layer width	-	50
Activation function	ELU	LeakyReLU
Activation func. par.	1 (scale)	0.03 (neg. slope)
Max epochs	5,000	50,000
Max # frames	100,000	1,000,000

the target metric stops improving according to the *ReduceLROnPlateau* scheduler (LRS). For agent exploration we employ the ϵ -greedy scheme. The list of optimizable parameters along with their distributions and environment-specific bounds is given in Table F.3.

Regarding the choice of the weight c in Equation 15, the approach we took was to first train agents without the convexity loss and then to evaluate their convexity losses with respect to a convexity measure of choice. c is then chosen such that the TD-MSE and the average convexity MSE loss are roughly equal. Future work can investigate this topic further, for a more systematic and general handling of this parameter, potentially providing even better performance enhancements.

Parameter	Distribution	Tiger bounds	FVRS bounds
Initial learning rate	log-uniform	$[e^{-4}, e^{-1}]$	$[e^{-7}, e^{-3}]$
Replay buffer size	int-uniform	$[1, 10^5]$	$[1, 10^6]$
# epochs per rollout	int-uniform	[1, 25]	[1, 25]
LRS factor	uniform	[0.8, 1.0]	[0.8, 1.0]
LRS patience	int-uniform	$[1, 10^4]$	$[1, 5 \cdot 10^4]$
# ϵ steps	int-uniform	$[1, 10^4]$	$[1, 10^5]$
Final ϵ	uniform	[0.001, 0.5]	[0.001, 0.5]